PH5490: PS01 Instructor: Rajesh Singh (rsingh@smail.iitm.ac.in)

1. **Principle of Maximum Entropy.** The Gibbs entropy [1] is defined as:

$$S = -k_B \sum_i p_i \ln p_i \tag{1}$$

Here p_i is the the probability of the ith state. This is also called the Shannon entropy (without the k_B factor). The system also has some constraints such as:

$$\sum_i p_i = 1, \qquad \sum_i p_i \phi_i^\alpha = \bar{\phi}^\alpha$$

The first constraint is simply the normalisation of the probability, while the second constraint may correspond to, for example, in canonical ensemble for a constant energy etc. Here ϕ_i^α is a variable, which could be the energy of the ith state. Use the Gibbs form of entropy and constraints along with Lagrange's method of undetermined multipliers to obtain probability distribution function (PDF) in all the three ensembles from statistical mechanics: (a) Microcanonical, (b) Canonical, (c) Grand-canonical.

2. **Avatars of entropy**. Find the equivalence:

   (a) In 1865, Clausius defined entropy S as: $dS = \delta Q/T$.

   (b) The Boltzmann entropy: $S = k_B \ln \Omega$. Here Ω is the total number of states.

   (c) The Gibbs entropy: $S = -k_B \sum_i p_i \ln p_i = -k_B \langle \ln p \rangle$.

3. **Gaussian integrals**. Prove the following

$$I = \int_{-\infty}^{\infty} e^{-ax^2}\, dx = \sqrt{\frac{\pi}{a}} \tag{2}$$

This result can be derived by considering I^2 and then doing the integration in plane polar coordinates r, θ. Use the above result to obtain:

$$\int_{-\infty}^{\infty} e^{-ax^2+bx}\, dx = \sqrt{\frac{\pi}{a}} \exp\left(\frac{b^2}{4a}\right). \tag{3}$$

Use the above to prove (hint: apply $\frac{\partial}{\partial b}$ repeatedly...):

$$\int_{-\infty}^{\infty} x\, e^{-ax^2+bx}\, dx = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{4a}}\, \frac{b}{2a}, \qquad \int_{-\infty}^{\infty} x^2\, e^{-ax^2+bx}\, dx = \sqrt{\frac{\pi}{a}}\, e^{\frac{b^2}{4a}} \left[\frac{b^2}{4a^2} + \frac{1}{2a}\right]$$

4. **Random walks in 1D.** Consider the random walk in 1D. Each steps can be to the right or left is of length l. Displacement after N steps is

$$x = l \sum_i \sigma_i, \qquad \sigma_i = \pm 1. \tag{4}$$

   (a) Find the average displacement $\langle x \rangle$.

   (b) Find the MSD (mean-squared-displacement) $\langle x^2 \rangle$ using $\langle \sigma_i \sigma_j \rangle = \delta_{ij}$.

   (c) Show that the probability that the walker ends at $x = ml$ after N steps is:

$$p(m) = \frac{\Omega(m)}{2^N}, \qquad \Omega(m) = \frac{N!}{\left[\frac{1}{2}(N-m)\right]! \, \left[\frac{1}{2}(N+m)\right]!} \tag{5}$$

   (d) Compute and plot entropy $S(x)$ using the Boltzmann formula of entropy: $S = k_B \ln \Omega$. You may use the Stirling's approximation $\ln(N!) = N \ln N - N + O(\ln N)$ in the limit of $N \to \infty$. What is the maximum value of the entropy.

   (e) Write the master equation of the random walk?

   (f) Using the master equation and Taylor expansion in the limit of small jump size and time steps Δt), show that the probability distribution follows:

$$\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p(x,t)}{\partial x^2}, \qquad D = \frac{l^2}{2\Delta t} \tag{6}$$

   (g) Solve the above Fokker-Planck equation for a delta function source $p(x, 0) = \delta(x)$.

   (h) Use the solution for the probability distribution to obtain mean position and the MSD. Compare with results in (a) and (b).

5. **Stable distributions and the central limit theorem**

   (a) What are stable probability distributions? What probability distribution you get on summing two uniformly distributed random variables?

   (b) The Gaussian distribution is given as:

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \tag{7}$$

      i. Find the mean μ and variance σ and obtain thee character function $\tilde{p}(k)$, defined as $\tilde{p}(k) = \int_{-\infty}^{\infty} dx \, p(x) \, e^{-ikx}$, of the above.

   (c) State and prove the central limit theorem [2]

6. **Master equation in Markovian systems.** A Markov process describes a sequence of possible stochastic events in which the probability of each event depends only on the state attained in the previous event. We consider a Markovian system with discrete states C_i, $i = 1, 2, 3, \ldots$ [3]. The probability $p(C_i)$ of finding the systems in the configuration C_i at time t evolves in time as

$$\frac{\partial p(C_i, t)}{\partial t} = \left[\sum_{i \neq j} \Pi_{ji}\, p(C_j, t) - \sum_{i \neq j} \Pi_{ij}\, p(C_i, t)\right] = \sum_{i \neq j} J_{ij}(t) \tag{8}$$

Here Π_{ij} is the rate of transition from configuration C_i to C_j. In other words, $\Delta t\, \Pi_{ij}$ is the the probability that in a small time Δt, the system changes from C_i to C_j.

(a) Explain the detailed-balance condition: $J_{ij} = 0$ or $\Pi_{ji}\, p_j = \Pi_{ij}\, p_i$.

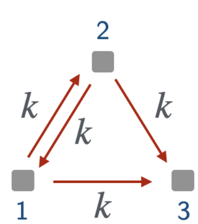
(b) Show the a necessary and sufficient condition for the detailed balance to hold is the Kolmogorov loop condition: $\Pi_{12}\, \Pi_{23} \ldots \Pi_{k1} = \Pi_{1k} \ldots \Pi_{32}\, \Pi_{21}$.

(c) Consider a system having only three possible states of the same energy. It can jump between states 1 and 2 and between states 2 and 3 but not directly between states 1 and 3. All jumps are at the same rate π_0. Show that the master equation is of the form (here $\mathbf{p} = (p_1, p_2, p_3)$):

$$\dot{\mathbf{p}} = \mathbf{\Pi} \cdot \mathbf{p}, \qquad \mathbf{\Pi} = \begin{bmatrix} -1 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -1 \end{bmatrix}. \tag{9}$$

Confirm that the probability in the equilibrium state is: $\mathbf{p}_{\text{eqm}} = (1, 1, 1)/3$.

7. Consider a system of 3 states (see Figure below). Here, all allowed transition between the states happen at rate k. If the system reaches state 3, then it remains there forever. The state 3 is said to be an absorbing state. Answer the following assuming that the system was prepared in state 1 at time $t = 0$.



(a) Write the Master equation for the evolution of the probability $p_1(t)$, $p_2(t)$ and $p_3(t)$ of the three states. Assume that state 3 is an absorbing state.

(b) Find the survival probability $S(t)$ for this system. $S(t)$ is defined as the probability that the system has not reached the absorbing state. Here, it is:

$$S(t) = \sum_{n \neq 3} p_n(t) = p_1(t) + p_2(t). \tag{10}$$

(c) Find the mean-first-passage time t_p, which is defined as: $t_p = \int_0^\infty S(t)\, dt$.

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[1] One can read more on this idea in E. T. Jaynes, *Probability Theory: The Logic of Science.*

[2] Read more on central limit theorem and universality at terrytao.wordpress.com/2010/09/14/a-second-draft-of-a-non-technical-article-on-universality.

[3] A Markov process with discrete states is called a Markov chain.